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Unravelling the role of Nickel doping on the physical properties of CuO thin films deposited by Spray Pyrolysis and theoretical analysis of nanostructured ZnO/Ni:CuO-based heterojunction solar cells

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Supplementary Information

3.2 Theoretical

SCAPS-1D software tool

- In this work a one-dimensional solar cell capacitance software (SCAPS-1D) developed by the University of Gent, Belgium is used.
- The Poisson and continuity equations for holes and electrons are as follows:

$$\frac{d}{dx}(\varepsilon(x)\frac{d\psi}{dx}) = q[p(x) - n(x) + N_D^+(x) - N_A(x) - p_t(x) - n_t(x)] \tag{S1}$$

$$\frac{1}{J}\frac{\partial J_p}{\partial x} + R_p(x) - G(x) = 0 \tag{S2}$$

$$-\frac{1}{J}\frac{\partial J_n}{\partial x} + R_n(x) - G(x) = 0 \tag{S3}$$

Here, ε is the permittivity, q – charge of electron, ψ – electrostatic potential and n – electrons' concentration, p – free hole concentration, n_t – trapped electron, p_t – trapped hole, N_D^+ – ionized donor like doping and N_A^- – ionized acceptor like doping concentrations, $R_n(x)$, $R_p(x)$ are electrons and holes recombination rates, $G(x)$ is the generation rate, J_n and J_p are the electron and hole current densities, respectively.

Solar cell performance

The measure of a photovoltaic cell quality is the Fill Factor (FF). $FF$is premeditated by equating the maximum power (P_{max}) to the theoretical power (P_t) which would be output at both the short circuit current (J_{sc}) and the open circuit voltage (V_{oc}) as given in equation *S*4. The ratio of the energy output from the photovoltaic solar cell to the energy input from the sun is the power conversion efficiency (PCE) mathematically expressed in equation *S*5.

$$FF = \frac{P_{max}}{P_t} = \frac{V_{max}I_{max}}{V_{oc}J_{sc}} \tag{S4}$$

$$PCE = \frac{V_{oc}J_{sc}FF}{P_{in}} \tag{S5}$$

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Table S 1: Materials parameters used in the simulation (Ahmmed et al., 2021)

Material properties	Unit	ITO	ZnO NRs	Ni:CuO
Thickness (μm)	μm	0.1	0.25	1.6
Relative dielectric permittivity (ε)	-	8.9	9	10
Band gap (E_g)	eV	3.65	3.37	Variable
Electron affinity (χ)	eV	4.5	4.2	4.07
CB effective density of states Nc	cm^{-3}	5.2×10^{18}	2.2×10^{18}	2.2×10^{19}
VB effective density of states Nv	cm^{-3}	1.1×10^{18}	1.8×10^{19}	5.5×10^{20}
Electron mobility (μ_e)	cm^2/V.s	40	200	10
Hole mobility (μ_h)	cm^2/V.s	30	50	0.1
Donor (Acceptor) density $N_{D(A)}$	cm^{-3}	1×10^{21}	1×10^{18}	1×10^{16}
Defect density	cm^{-3}		1×10^{17}	1×10^{18}

References

Ahmmed, S., Aktar, A., Tabassum, S., Rahman, M. H., Rahman, M. F., & Md. Ismail, A. B. (2021). CuO based solar cell with V2O5 BSF layer: Theoretical validation of experimental data. *Superlattices and Microstructures*, *151*, 106830. doi: doihttps://doi.org/10.1016/j.spmi.2021.106830